INTRODUCTION TO QUANTUM MECHANICS – ADVANCED EXAMPLES I

3RD LECTURE
FROM THE COURSE
QUANTUM PHYSICS OF LOW DIMENSIONAL STRUCTURES

QPLDS

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CONTENTS

THE WAVE-EQUATION FOR A MANY-BODY PROBLEM INCLUDING SPINS. THE PAULI PRINCIPLE and indistinguishable objects

Some conventions for

The wave-function (the physical state vector)

$$\Psi = \Psi(\vec{r}_1, s_1, \ldots, \vec{r}_N, s_N, t) \quad \rightarrow \quad \Psi = \Psi(1, \ldots, N, t)$$

Hamiltonian

$$H = H(\vec{r}_1, \vec{p}_1, s_1, \ldots, \vec{r}_N, \vec{p}_N, s_N, t) \quad \rightarrow \quad H = H(1, \ldots, N, t)$$

Physical particles in low-dimensional structures should be indistinguishable

The operator of reorder P_{ik}

$$\boxed{P_{ik}\Psi(1, \ldots, i, \ldots, k, \ldots, \ldots N, t) = \Psi(1, \ldots, k, \ldots, i, \ldots, \ldots N, t)}$$

Particles can not be recognized from their interactions described by the Hamiltonian

$$\boxed{[P_{ik}, H] = 0}$$

the proof

$$P_{ik} H(i,k)\Psi(i,k) = H(k,i)\Psi(k,i) = H(k,i)P_{ik}\Psi(i,k)$$

$$P_{ik} H(i,k) = H(k,i)P_{ik} \quad \Rightarrow \quad P_{ik} H(i,k) - H(k,i)P_{ik} = 0$$

The probability density can not be changed after exchanging particles states

(in a general case $\Psi(i,k) = \lambda\Psi(k,i), \quad \lambda = const$)

The eigen-problem for the reorder operator

$$\boxed{P_{ik}\Psi(i,k) = \lambda\Psi(i,k)}$$

$$P_{ik}\Psi(i,k) = \lambda\Psi(i,k) \ \ / P_{ik}$$

$$P_{ik}^2\Psi(i,k) = \lambda P_{ik}\Psi(i,k) \qquad\qquad P_{ik}^2 = I$$

$$\Psi(i,k) = \lambda^2\Psi(i,k) \quad \Rightarrow \quad \lambda^2 = 1, \quad \lambda = \pm 1$$

Conclusion_1: the eigen-problem for the reorder operator has two possibilities

$$P_{ik}\Psi(i,k)=\Psi(i,k) \text{ and } P_{ik}\Psi(i,k)=-\Psi(i,k)$$

Conclusion_2: as we assumed that $\Psi(i,k)=\lambda\Psi(k,i)$, then wave-function can be in general symmetrical and/or anti-symmetrical

$$\boxed{\Psi(i,k)=\pm\Psi(k,i)}$$

THE IMPORTANT ISSUE

THE SCHRÖDINGER EQUATION HAS THE SAME SYMMETRY AS THE WAVE-VECTOR

$$H\Psi=-\frac{\hbar}{i}\frac{\partial\Psi}{\partial t}$$

in other words, when Ψ possesses a given symmetry, then $\partial\Psi/\partial t$ adopts this symmetry, thus, the $H\Psi$ term has the same symmetry.

It is true for a given moment
but,
is it true for all times?

$$\Psi(t+dt)=\Psi(t)+\frac{\partial\Psi}{\partial t}dt$$

The symmetry of a wave-function does not change in time

Some remarks related to electrons

$$\Psi_{k_1,k_2,\ldots,k_N}(1,2,\ldots,N,t)=-\Psi_{k_1,k_2,\ldots,k_N}(2,1,\ldots,N,t)$$

$$\Psi_{k_1,k_2,\ldots,k_N}(1,2,\ldots,N,t)=-\Psi_{k_2,k_1,\ldots,k_N}(1,2,\ldots,N,t)$$

thus

$$\Psi_{k_1,k_1,\ldots,k_N}(1,2,\ldots,N,t)=-\Psi_{k_1,k_1,\ldots,k_N}(2,1,\ldots,N,t)$$

$$\Psi_{k_1,k_1,\ldots,k_N}(1,2,\ldots,N,t)=\Psi_{k_1,k_1,\ldots,k_N}(2,1,\ldots,N,t)$$

PAULI PRINCIPLE

$$\Psi_{k_1,k_1,\ldots,k_N}(1,2,\ldots,N,t)\equiv 0 \qquad k_i=\{n_i,l_i,m_i,s_i\}$$

There are no two electrons being in the same state defined by the same set of quantum numbers

THE EXAMPLE OF THE TWO NOT INTERACTING ELECTRONS

In the first lecture following SPIN-like functions were introduced

$$\chi_{1/2}(1)\chi_{1/2}(2) \quad \chi_{1/2}(1)\chi_{-1/2}(2) \quad \chi_{-1/2}(1)\chi_{1/2}(2) \quad \chi_{-1/2}(1)\chi_{-1/2}(2)$$

plus their symmetrical and anti-symmetrical combinations:

symmetrical

$$\chi_{1/2}(1)\chi_{1/2}(2)$$

$$\chi_{-1/2}(1)\chi_{-1/2}(2)$$

$$\frac{\sqrt{2}}{2}[\chi_{1/2}(1)\chi_{-1/2}(2)+\chi_{-1/2}(1)\chi_{1/2}(2)]$$

anti-symmetrical

$$\frac{\sqrt{2}}{2}[\chi_{1/2}(1)\chi_{-1/2}(2)-\chi_{-1/2}(1)\chi_{1/2}(2)]$$

The SPACE-like two-body wave-functions (for arbitrary electrons i and k, where i and k in fact mean sets of quantum numbers) they can be

$\Psi_i(\vec{r}_1)\Psi_k(\vec{r}_2)+\Psi_k(\vec{r}_1)\Psi_i(\vec{r}_2)$ (SYMMETRICAL)

$\Psi_i(\vec{r}_1)\Psi_k(\vec{r}_2)-\Psi_k(\vec{r}_1)\Psi_i(\vec{r}_2)$ (ANTI-SYMMETRICAL)

HOWEVER, we look for the total wave-function including space and spin components.

There are following possibilities (ANTI-SYMMETRICAL):

TRIPLET STATES

$$1/\sqrt{2}[\Psi_i(\vec{r}_1)\Psi_k(\vec{r}_2)-\Psi_k(\vec{r}_1)\Psi_i(\vec{r}_2)]\chi_{1/2}(1)\chi_{1/2}(2) \quad \uparrow\uparrow$$

$$1/\sqrt{2}[\Psi_i(\vec{r}_1)\Psi_k(\vec{r}_2)-\Psi_k(\vec{r}_1)\Psi_i(\vec{r}_2)]\chi_{-1/2}(1)\chi_{-1/2}(2) \quad \downarrow\downarrow$$

$$1/2[\Psi_i(\vec{r}_1)\Psi_k(\vec{r}_2)-\Psi_k(\vec{r}_1)\Psi_i(\vec{r}_2)][\chi_{1/2}(1)\chi_{-1/2}(2)+\chi_{-1/2}(1)\chi_{1/2}(2)] \quad \uparrow\downarrow\uparrow\downarrow$$

THE SINGLET STATE

$$1/2[\Psi_i(\vec{r}_1)\Psi_k(\vec{r}_2)+\Psi_k(\vec{r}_1)\Psi_i(\vec{r}_2)][\chi_{1/2}(1)\chi_{-1/2}(2)-\chi_{-1/2}(1)\chi_{1/2}(2)] \quad \uparrow\downarrow$$

THE EXAMPLE OF THE OVER-SUBTLE ENERGY SPLITTING IN THE HYDROGEN ATOM

The splitting can results from the dipole-type (long range) interaction between the electron-spin and the proton-spin located in the atomic nucleus.

The energy operator (the Hamiltonian)

$$H = A\hat{\sigma}^{el}\hat{\sigma}^{p} = A(\hat{\sigma}_1^{el}\hat{\sigma}_1^{p} + \hat{\sigma}_2^{el}\hat{\sigma}_2^{p} + \hat{\sigma}_3^{el}\hat{\sigma}_3^{p})$$

The base vectors to describe this phenomenon (this is the Hilbert space) are

$$\chi_{-1/2}(el)\chi_{-1/2}(p) \quad \chi_{-1/2}(el)\chi_{1/2}(p) \quad \chi_{1/2}(el)\chi_{-1/2}(p) \quad \chi_{1/2}(el)\chi_{1/2}(p)$$

Let’s introduce new descriptions:

$$\chi_{-1/2}(el)\chi_{-1/2}(p) = |1>$$

$$\chi_{-1/2}(el)\chi_{1/2}(p) = |2>$$

$$\chi_{1/2}(el)\chi_{-1/2}(p) = |3>$$

$$\chi_{1/2}(el)\chi_{1/2}(p) = |4>$$

and calculate the Hamiltonian in this base:

$$H_{ik} = < i \,|\, H \,|\, k >= A < i \,|\, \hat{\sigma}^{el} \hat{\sigma}^{p} \,|\, k >, \quad i,k = 1,2,3,4$$

$$H_{ik} = A < i \,|\, \hat{\sigma}^{el} \hat{\sigma}^{p} \,|\, k >= \begin{bmatrix} A & 0 & 0 & 0 \\ 0 & -A & 2A & 0 \\ 0 & 2A & -A & 0 \\ 0 & 0 & 0 & A \end{bmatrix}$$

Above matrix was derived using $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ matrixes for the base vectors.

For example

$$A\sigma_x^{el}\sigma_x^{p}(p)\chi_{1/2}(el)\chi_{1/2}(p) = A\sigma_x^{el}\chi_{1/2}(el)\sigma_x^{p}\chi_{1/2}(p) =$$
$$= A\chi_{-1/2}(el)\chi_{-1/2}(p) = A$$

Thus, the eigen-equation (equation of “motion”) has the following form

$$\begin{bmatrix} A & 0 & 0 & 0 \\ 0 & -A & 2A & 0 \\ 0 & 2A & -A & 0 \\ 0 & 0 & 0 & A \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix} = E \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \end{bmatrix}$$

or in the compact form

$$\sum_k H_{ik}\alpha_k = E^{(i)}\alpha_i$$

From that results the condition of unique solution

$$\det\begin{bmatrix} A-E & 0 & 0 & 0 \\ 0 & -A-E & 2A & 0 \\ 0 & 2A & -A-E & 0 \\ 0 & 0 & 0 & A-E \end{bmatrix} = 0,$$

then, result the following eigen-values

$E^{(1)} = E^{(3)} = E^{(4)} = A$ for a degenerated triplet state,
$E^{(2)} = -3A$ for a nondegenerated singlet state,

and the respective eigen-vectors look as follows:

$$\alpha^{(1)} = \chi_{-1/2}(el)\chi_{-1/2}(p)$$

$$\alpha^{(3)} = \frac{\sqrt{2}}{2}(\chi_{-1/2}(el)\chi_{1/2}(p) + \chi_{1/2}(el)\chi_{-1/2}(p))$$

$$\alpha^{(4)} = \chi_{1/2}(el)\chi_{1/2}(p)$$

$$\alpha^{(2)} = \frac{\sqrt{2}}{2}(\chi_{-1/2}(el)\chi_{1/2}(p) - \chi_{1/2}(el)\chi_{-1/2}(p))$$

Conclusion: Hydrogen in the ground state can be in a triplet state (J=1, M=-1, 0, 1) OR in the singlet state (J=0, M=0).

Next, the energy diagram for the all states looks as follows

ν=1420405751.8 *Hz*